THE CCP13 RA, Dr. RICHARD DENNY - A PROFILE

Richard Denny graduated from Keele in 1986 in mathematics and physics. Postgraduate work was also carried out at Keele into structural transitions in the conformationally flexible DNA double-helix using X-ray fibre diffraction, under the guidance of Professor Watson Fuller.

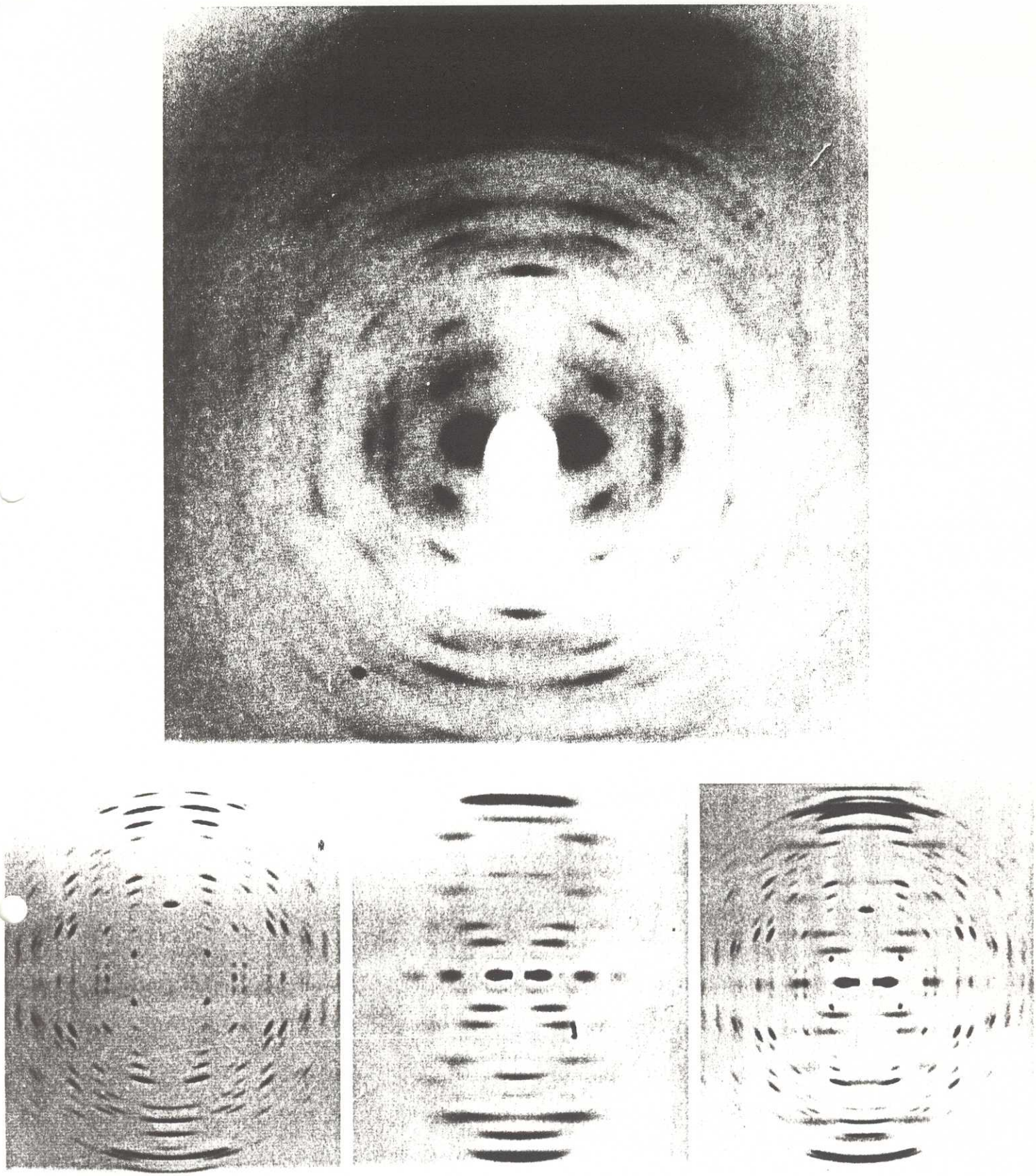
The main area of study was the S -> B transition where the DNA double-helix is thought to change handedness from left to right. One of the approaches adopted was to simulate fibre diffraction patterns using the two end point structures, incorporating various types of lattice disorder (see Figures on Page 9).

In October 1990, allegiance was switched within the Keele physics department, to the protein crystallography group run by Trevor Greenhough. Here, the majority of work involved carrying out and analyzing the results of multi-wavelength anomalous diffraction (MAD) experiments using CCP4 programs and a suite of programs specific to MAD data analysis supplied by Wayne Hendrickson.

Two systems were studied, oligopeptide permease A(oppA) and an 18 kDalton fragment of duck ovo-transferrin (dOT) using station 9.5 at the SRS. Other work has included conversion of the Laue integration program INTLAUE for use with image plates and the simulation of thermal diffuse scatter using correlations derived from molecular dynamics simulations.

Current work for CCP13 includes the modification and updating of a fibre diffraction package whose authors include Colin Nave, Richard Bryan and Ian Clifton. The package is designed to remove background and assign intensities to Bragg spots or evaluate continuously varying intensity along layer lines by a maximum entropy method, which depends on calculating expected profiles for spots or layer line broadening.

Richard Denny started as the CCP13 RA on October 1st, 1992 and currently spends Monday to Wednesday each week at Daresbury and Thursday & Friday at Imperial College, London. As the RA on this project, one of his briefs is to visit contributing Research Groups to get first hand experience of the problems that people are facing in their particular fibre diffraction studies so that the newly developed software package can be as useful as possible. Please contact him if you would like him to visit your Group.



The top photograph shows a frame recorded during time-resolved monitoring of the S to B transition in DNA. The predominant conformation appears to be S_{II}, but there is also strong equatorial intensity and other diffuse scatter not associated with S_{II}. Bottom left is a photograph of a pattern simulated from a model S_{II} structure. Bottom middle is a pattern simulated from a B model with slippage disorder and paracrystallinity (distortions of the 2nd kind). Bottom right shows the addition of these simulations in the ratio 50 B : 1 S_{II}.